

A recursive approach to determine correlation functions in multi-baryon systems

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We propose a recursive algorithm for the calculation of multi-baryon correlation functions that combines the advantages of a recursive approach with those of the recently proposed unified contraction algorithm. The independent components of the correlators are built recursively by adding the baryons one after the other in a given order. The list of nonzero independent components is also constructed in a recursive manner, significantly reducing the resources required for this step. We computed the number of operations required to calculate the correlators up to ${}^8\text{Be}$, and observed a significant speedup compared to other techniques. For the calculation of ${}^4\text{He}$ and ${}^8\text{Be}$ correlation functions in the fully relativistic case $\mathcal{O}(10^8)$ operations are required, whereas for non-relativistic operators this number can be reduced to e.g. $\mathcal{O}(10^4)$ in the case of ${}^4\text{He}$.

1 Introduction

Quantum Chromodynamics (QCD), the theory of the strong interaction was first introduced to describe the strong nuclear binding forces. Given this fact QCD is expected to be able to predict the masses and properties of atomic nuclei. Due to the strong coupling at low energies non-perturbative techniques such as lattice QCD (LQCD) are required to study bound states in QCD. In principle the tools for such studies are at hand and several calculations in order to examine light nuclei [1–3] and the nuclear force [4–6] have been performed recently. However, the enormous amount of Wick-contractions

necessary for the evaluation of correlation functions of atomic nuclei is a severe problem in such calculations.

The number of Wick-contractions for the naïve evaluation of correlation functions of multi-baryon systems scales as $n_u! n_d! n_s!$, where n_u , n_d and n_s are the number of u , d and s quarks in the system, respectively. Furthermore, for each Wick-contraction one has to evaluate the sum over all color and spin indices. These sums scale exponentially with the number of baryons in the system. As a consequence, the total number of required operations scales as $n_u! n_d! n_s! 6^A 4^A$, where A is the atomic mass number. The introduction of more complicated spatial baryonic wave-functions will increase this number further.

Recently there has been substantial progress in reducing this computational challenge. An algorithm proposed in Ref. [7] reduces the computational cost by transforming the factorially scaling task of calculating Wick-contractions into the polynomially scaling task of calculating determinants. In [1] the number of contractions has been reduced significantly by exploiting the permutation symmetry of the quark operators. A further improvement has been achieved in [8], where the combined permutations of color and spin indices are used to create a unified list of independent contractions. While this method reduces the amount of contractions to be evaluated on each gauge configuration significantly, the creation of the list of independent contractions remains difficult. This is due to the fact that the full set of possible contractions, which scale factorially and exponentially in the number of quarks, has to be applied once to determine the coefficients in the list. For small systems it is possible to carry out this calculation once, but it becomes quickly impractical for larger systems.

For the related case of systems comprised of a large number of mesons recursive relations were derived in Ref. [9], which expose linear scaling for a fixed number of sources and polynomial behavior in the number of sources. The generalization of this method to systems of protons and neutrons is possible and results in a procedure which can be shown to scale polynomially in the number of nucleons and exponentially in the number of quark sources. Such an approach has the disadvantage that the resulting recursion relations are relatively complicated. Furthermore, the projection of the individual baryons to definite momentum or the introduction of additional quark sources remains difficult.

The purpose of this paper is to propose an efficient method for the calculation of baryonic correlation functions of the form

$$[C^{(N)}]_{\alpha_1 \alpha_2 \dots \alpha_N}^{\alpha'_1 \alpha'_2 \dots \alpha'_N}(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N, t) = \left\langle \prod_{k=1}^N B_{\alpha_k}(\vec{x}_k, t) \prod_{l=1}^N \bar{B}^{\alpha'_l}(\vec{0}, 0) \right\rangle \quad (1.1)$$

that combines the advantages of the recursive approach with those of the algorithm

introduced in [8]. The interpolating baryon operators are of the form

$$B_\alpha = \varepsilon_{abc} (\Gamma_1)_{\alpha\beta} (q_1)_{\beta;a} [(q_2)_{\gamma;b} (\Gamma_2)_{\gamma\delta} (q_3)_{\delta;c}], \quad (1.2a)$$

$$\bar{B}^\alpha = \varepsilon^{abc} (\Gamma_1)^{\alpha\beta} (\bar{q}_1)^{\beta;a} [(\bar{q}_2)^{\gamma;b} (\Gamma_2)^{\gamma\delta} (\bar{q}_3)^{\delta;c}], \quad (1.2b)$$

where the quark operators $q_n \in \{u, d, s\}$ and $\bar{q}_n \in \{\bar{u}, \bar{d}, \bar{s}\}$ are all taken at the same spacetime point. Here and throughout in the paper Latin indices correspond to color degrees of freedom (DoFs) while Greek indices correspond to the spin DoFs associated with the quark operators. For notational convenience all upper indices correspond to quark operators at the source while lower indices correspond to quark operators at the sink. The choice of $\Gamma_1 = \mathbf{1}$ and $\Gamma_2 = C\gamma_5$ yields the interpolating operators for the proton with $(q_1, q_2, q_3) = (u, u, d)$ and for the neutron with $(q_1, q_2, q_3) = (d, u, d)$.

The paper is organized as follows. First we review the unified contraction algorithm in Section 2. In Section 3 a method is introduced to construct antisymmetric tensors out of small building blocks in a recursive way. This procedure is applied in Section 4 to construct correlation functions of multi-baryon systems with one quark source and one baryon sink. In Section 5 a method is described to reduce the number of necessary operations when only the projection of the correlation function to a certain angular momentum state is of interest. This is followed by the generalization of the method to an arbitrary number of quark sources and baryon sinks in Section 6, which allows the calculation of arbitrarily complex correlation functions. The case of atomic nuclei is discussed in detail in Section 7. Finally, after comparing the efficiency of our method with that of other recent algorithms in Section 8 we conclude in Section 9.

2 The unified contraction algorithm

To provide a self-contained presentation, we briefly review in this section the unified contraction algorithm introduced in Ref. [8]. For the construction of multi-baryon correlation functions it is useful to define blocks of quark propagators which correspond to the contractions of three quarks at the source with a baryon at the sink. This blocking procedure, which was successfully used both for the study of light nuclei [1–3] and for the study of several-nucleon forces [4–6], has several advantages. First it already reduces the number of contractions to evaluate. Second it allows to carry out the projection of individual baryons to definite momentum or to introduce different baryon sinks prior to the expensive calculation of the correlation function. The blocks are generally defined as

$$f_B^{q_1, q_2, q_3}(t, \delta; \alpha, \beta, \gamma; a, b, c) = \sum_{\vec{x}} s(\vec{x}) \left\langle B_\delta(\vec{x}, t) \cdot q_1^{\alpha;a} q_2^{\beta;b} q_3^{\gamma;c} \right\rangle. \quad (2.1)$$

Here δ is the spin index of the baryon B , α, β and γ are the spin indices of the three quarks q_1, q_2 and q_3 , and a, b, c are the corresponding color indices. The form of all three quark source operators are taken to be the same. The function $s(\vec{x})$ characterizes

the form of the baryon sink. A common choice is the projection to zero momentum $s(\vec{x}) \propto 1$, which is often needed e.g. when the mass of a bound state is to be extracted from a correlation function. For the moment it is assumed that the sink function is the same for all baryons and the case of different sinks is discussed later. For notational convenience the 4 spinor and 3 color degrees of freedom associated with a quark of a given flavor can be combined to form spinor-color indices $\xi^{(q)}$, which can take the values 1, 2, ..., 12. Using these combined indices a block can be written as

$$f_B^{q_1, q_2, q_3}(t, \delta; \xi^{(q_1)}, \xi^{(q_2)}, \xi^{(q_3)}) = \sum_{\vec{x}} s(\vec{x}) \left\langle B_\delta(\vec{x}, t) \cdot q_1^{\xi^{(q_1)}} q_2^{\xi^{(q_2)}} q_3^{\xi^{(q_3)}} \right\rangle. \quad (2.2)$$

In the case of a system consisting of protons $q_1 = q_2 = u$, therefore, the above tensor is antisymmetric in the indices $\xi^{(q_1)}$ and $\xi^{(q_2)}$.

Using the above defined blocks the correlation function of N baryons can be expressed as¹

$$\begin{aligned} [C^{(N)}]_{\delta_1, \delta_2, \dots, \delta_N}^{\alpha_1, \alpha_2, \dots, \alpha_N}(t) = & \sum_{\sigma \in \Sigma} f_{B_1}^{q_1, q_2, q_3}(t, \delta_1; \xi_1^{(q_1)}, \xi_2^{(q_2)}, \xi_3^{(q_3)}) \dots f_{B_N}^{q_1, q_2, q_3}(t, \delta_N; \xi_{3N-2}^{(q_1)}, \xi_{3N-1}^{(q_2)}, \xi_{3N}^{(q_3)}) \\ & \cdot G^{B_1}(\alpha_1; \xi_{\sigma(1)}^{(q_1)}, \xi_{\sigma(2)}^{(q_2)}, \xi_{\sigma(3)}^{(q_3)}) \dots G^{B_N}(\alpha_N; \xi_{\sigma(3N-2)}^{(q_1)}, \xi_{\sigma(3N-1)}^{(q_2)}, \xi_{\sigma(3N)}^{(q_3)}) \operatorname{sgn}(\sigma), \end{aligned} \quad (2.3)$$

where the objects G_B are combinations of Γ -matrices and ε -tensors suitable for a baryon B :

$$G^B(\alpha; \xi^{(q_1)}, \xi^{(q_2)}, \xi^{(q_3)}) := (\Gamma_1)^{\alpha \beta(\xi^{(q_1)})} (\Gamma_2)^{\beta(\xi^{(q_2)}) \beta(\xi^{(q_3)})} \varepsilon^{c(\xi^{(q_1)}) c(\xi^{(q_2)}) c(\xi^{(q_3)})}. \quad (2.4)$$

Here $\beta(\xi)$ is the spin-index part of ξ and $c(\xi)$ is the color-index part and Σ is the set of all permutations that permute the indices associated with the different quark flavors q_k separately. The product of blocks $f_B^{q_1, q_2, q_3}$ does not depend on the permutations σ and hence the correlation function can be written in the form

$$\begin{aligned} [C^{(N)}]_{\delta_1, \delta_2, \dots, \delta_N}^{\alpha_1, \alpha_2, \dots, \alpha_N}(t) = & f_{B_1}^{q_1, q_2, q_3}(t, \delta_1; \xi_1^{(q_1)}, \xi_2^{(q_2)}, \xi_3^{(q_3)}) \dots f_{B_N}^{q_1, q_2, q_3}(t, \delta_N; \xi_{3N-2}^{(q_1)}, \xi_{3N-1}^{(q_2)}, \xi_{3N}^{(q_3)}) \\ & \cdot L^{(N)}(\alpha_1, \dots, \alpha_N; \xi_1^{(q_1)}, \xi_2^{(q_2)}, \xi_3^{(q_3)}, \dots, \xi_{3N-2}^{(q_1)}, \xi_{3N-1}^{(q_2)}, \xi_{3N}^{(q_3)}) \end{aligned} \quad (2.5)$$

with the tensor

$$\begin{aligned} L^{(N)}(\alpha_1, \dots, \alpha_N; \xi_1^{(q_1)}, \xi_2^{(q_2)}, \xi_3^{(q_3)}, \dots, \xi_{3N-2}^{(q_1)}, \xi_{3N-1}^{(q_2)}, \xi_{3N}^{(q_3)}) = & \sum_{\sigma \in \Sigma} G^{B_1}(\alpha_1; \xi_{\sigma(1)}^{(q_1)}, \xi_{\sigma(2)}^{(q_2)}, \xi_{\sigma(3)}^{(q_3)}) \dots G^{B_N}(\alpha_N; \xi_{\sigma(3N-2)}^{(q_1)}, \xi_{\sigma(3N-1)}^{(q_2)}, \xi_{\sigma(3N)}^{(q_3)}) \operatorname{sgn}(\sigma). \end{aligned} \quad (2.6)$$

In the unified contraction algorithm the object L is generated by explicitly performing all

¹We use the Einstein summation convention throughout the paper, that is, over each index appearing twice the sum is automatically understood.

permutations according to eqn. (2.6). Since the G_B 's are very sparsely populated tensors in most cases L is also sparse. It is then proposed to consider only those components of the product $f_{B_1}^{q_1, q_2, q_3} \dots f_{B_N}^{q_1, q_2, q_3}$ which are contracted with the non-zero components of L .

3 Recursive construction of antisymmetric tensors

The object L has a high degree of symmetry which reduces the number of its independent components. From the definition it is straightforward to see that L is antisymmetric under the exchange of two indices ξ as long as they belong to the same quark flavor. It also possesses a number of spin indices $\alpha_1 \dots \alpha_N$ corresponding to baryons of types B_1, B_2, \dots, B_N . From the Pauli-principle it follows that the correlator $[C^{(N)}]_{\delta_1, \delta_2, \dots, \delta_N}^{\alpha_1, \alpha_2, \dots, \alpha_N}(t)$ has to be antisymmetric under the exchange of any two indices α corresponding to the same type of baryon. Hence the same property has to hold for L .

It can be shown using only this antisymmetric property that the maximal number of independent components e.g. in the case of ${}^4\text{He}$ is 30735936, whereas in the case of ${}^8\text{Be}$ it is 1. Since the objects G are very sparse, many of these components are expected to be zero.

A component of a tensor $X(\xi_1, \xi_2, \dots, \xi_l)$, which is antisymmetric in the indices $\xi_1, \xi_2, \dots, \xi_l$, each ranging from 1 to k , can be uniquely defined by a k -tuple $\mathbf{A}\{\xi\} = (n(1), n(2), \dots, n(k))$, where $n(i)$ denotes how often the value i occurs amongst the l indices in the set $\{\xi\} = \{\xi_1, \xi_2, \dots, \xi_l\}$. As a consequence of the antisymmetry all components with $n(i) > 1$ vanish. The component associated with such a tuple is the component where all values i for which $n(i) = 1$ occur amongst the indices in ascending order. All other components can be constructed using permutations of the indices and taking the sign of the permutation into account. For example, if X is a tensor with three antisymmetric indices, each ranging from one to four, the tuple $\mathbf{A}\{\xi\} = (1, 0, 1, 1)$ corresponds to the component $X(1, 3, 4)$. If a tensor is antisymmetric in several groups of indices independently, then several independent tuples can be defined, one for each group of indices.

If X is an antisymmetric tensor with k indices and Y is an antisymmetric tensor with l indices, then their antisymmetric product $Z = X \bullet Y$ is a tensor with $k+l$ antisymmetric indices, whose components are defined as²

$$(X \bullet Y)(\mathbf{z}) := Z(\mathbf{z}) = \sum_{\mathbf{z}=\mathbf{x}+\mathbf{y}} X(\mathbf{x})Y(\mathbf{y}) \text{sgn}(\mathbf{x}|\mathbf{y}), \quad (3.1)$$

²In the definition of this product the normalization factors have been removed deliberately to speed up the computation. These factors will be reintroduced when the correlation function is calculated.

where the tuples

$$\mathbf{z} = \mathbf{A}\{\xi_1, \dots, \xi_{k+l}\} \quad (3.2)$$

$$\mathbf{x} = \mathbf{A}\{\xi_1, \dots, \xi_k\} \quad (3.3)$$

$$\mathbf{y} = \mathbf{A}\{\xi_{k+1}, \dots, \xi_{k+l}\} \quad (3.4)$$

identify the antisymmetric components and

$$\text{sgn}(\mathbf{x}|\mathbf{y}) = \prod_{\substack{i>j \\ y_j=1}} (-1)^{x_i} \quad (3.5)$$

is the sign of the permutation that is necessary to bring the indices of the tensors X and Y into ascending order.

If each tensor has r independent groups of antisymmetric indices then each such group is described by an individual tuple. In this case the antisymmetrized product can be written as

$$\begin{aligned} (X \bullet Y)(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_r) := \\ Z(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_r) = \sum_{\substack{\mathbf{z}_1=\mathbf{x}_1+\mathbf{y}_1 \\ \mathbf{z}_2=\mathbf{x}_2+\mathbf{y}_2 \\ \dots \\ \mathbf{z}_r=\mathbf{x}_r+\mathbf{y}_r}} X(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_r) Y(\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_r) \times \\ \times \text{sgn}(\mathbf{x}_1|\mathbf{y}_1) \text{sgn}(\mathbf{x}_2|\mathbf{y}_2) \dots \text{sgn}(\mathbf{x}_r|\mathbf{y}_r). \end{aligned} \quad (3.6)$$

In the following it will be often required to antisymmetrize only the subset of the quark color-spinor indices ξ that corresponds to a given quark flavor q . In this case it will be useful to write $\mathbf{A}^{(q)}\{\xi_1, \xi_2, \dots, \xi_n\}$ for the tuple of indices associated with the respective quark flavor. In the case of the spinor indices α and δ of the baryons a similar notation is adopted: here $\mathbf{A}^{(B)}\{\alpha_1, \alpha_2 \dots \alpha_n\}$ is the tuple associated with the antisymmetrization of only those spinor indices that correspond to the baryon type B .

In the special case where an antisymmetric tensor can be written as $X^{(n)} = Y_1 \bullet Y_2 \bullet \dots \bullet Y_n$, a recursion relation $X^{(i)} = X^{(i-1)} \bullet Y_i$ can be set up with the starting condition $X^{(1)} = Y_1$. The usage of this recursion relation is often much more efficient than the direct evaluation of the product $Y_1 \bullet Y_2 \bullet \dots \bullet Y_n$. Assuming that there are r groups of antisymmetric indices, each index in the p -th group can take values from 1 to m_p , and in the p -th group at the stage $X^{(i)}$ there are n_p indices, then the number of components at the intermediate step is

$$P^{(i)} = \prod_{p=1}^r C(n_p, m_p - n_p), \quad (3.7a)$$

where $C(n_1, n_2, \dots, n_m) = (n_1 + n_2 + \dots + n_m)! / n_1! n_2! \dots n_m!$ are the multinomial coef-

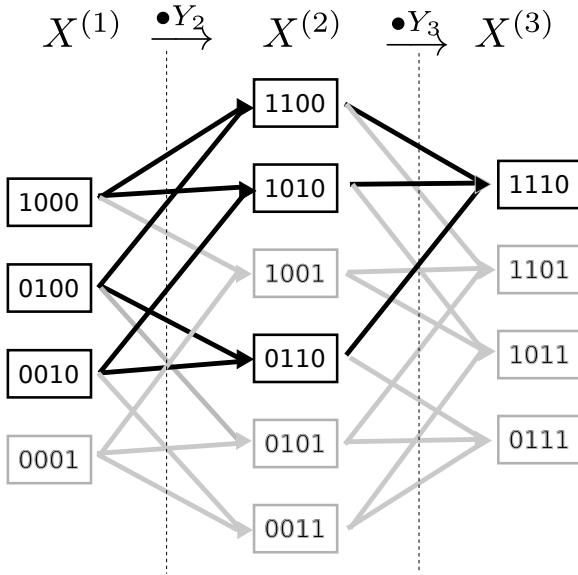


Figure 1: The computational savings of the recursive algorithm in the case when only one antisymmetric component of the result $X^{(3)}$ is of interest. $X^{(3)}$ has one group of antisymmetric indices, and each Y_i possesses only one index. The boxes in the three columns represent the antisymmetric components of the respective stages $X^{(1)}$, $X^{(2)}$ and $X^{(3)}$. The number in each box corresponds to the tuple associated with the antisymmetric component. The arrows show which components are used to construct the components of the next stage. If the gray boxes in the tensor $X^{(3)}$ are not needed, then the gray boxes in all other tensors are also not needed. Only the solid black operations have to be performed and the gray operations can be omitted.

ficients. The number of operations required to go from $X^{(i)}$ to $X^{(i+1)}$ is

$$Q^{(i)} = \prod_{p=1}^r C(n_p, l_p, m_p - n_p - l_p), \quad (3.7b)$$

where l_p is the number of indices in the p -th index group of Y_{i+1} .

A further reduction of the computational effort can be achieved when not all components of $X^{(n)}$ at the final stage are of interest. When evaluating the product $X^{(n)} = X^{(n-1)} \bullet Y_n$ only those summands have to be considered which contribute to a component of interest in $X^{(n)}$. Using this property not only the computational effort of evaluating this particular product can be reduced, but also some of the components of $X^{(n-1)}$ may not be required for the evaluation of the product at all. Therefore, these components of $X^{(n-1)}$ are not of interest and need not be computed in the previous recursion step. This argumentation can then be repeated for all recursion steps and often leads to a significant reduction of computational effort. The procedure is demonstrated in Figure 1 for the case where $X^{(n)}$ has only one group of antisymmetric indices, each index ranging from 1 to 4. The tensors Y_i here possess only one index of the same format. If it is assumed that at the final stage only the black component of $X^{(3)}$ is of interest then a significant reduction in the computational effort is achieved.

If it is known in advance which components of $X^{(n)}$ are of interest, then it is useful to determine which components of $X^{(n-1)}$ are required for their computation and to make a list $\Lambda^{(n-1)}$ of the required operations. This procedure can be repeated successively for all previous intermediate steps until $X^{(1)}$ is reached. For the computation of the desired

components of $X^{(n)}$ one then has to perform only the operations contained in the lists $\Lambda^{(1)}, \Lambda^{(2)}, \dots, \Lambda^{(n-1)}$.

In practice the lists $\Lambda^{(i)}$ are usually much larger than the tensors $X^{(i)}$. Therefore, the memory requirement of the resulting algorithm is dominated by these lists. This problem can be circumvented by storing at each stage i only the list of the required components of $X^{(i)}$. Then the reconstruction of the list of operations $\Lambda^{(i-1)}$ introduces a relatively small overhead, but the amount of memory used by the algorithm is reduced significantly.

4 Correlation functions with one quark source/sink

Using the notation from the previous section the tensor L can be written in the form³

$$L(\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \mathbf{A}^{(d)}\{\xi\}, \mathbf{A}^{(s)}\{\xi\}). \quad (4.1)$$

Here B_a, B_b, \dots are the different types of baryons in the system. Using a similar argumentation the object G^B can be written as

$$G^B(\alpha, \mathbf{A}^{(u)}\{\xi\}, \mathbf{A}^{(d)}\{\xi\}, \mathbf{A}^{(s)}\{\xi\}). \quad (4.2)$$

Although the index α is just a single spin index, it can be expressed through 4-tuples $\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \dots$ to bring G^B into the same form as L . Out of these tuples only the one corresponding to the baryon B will have a single nonzero entry.

The tensors $L^{(n)}$ defined in eqn. (2.6) corresponding to n baryons fulfill the recursion relation

$$L^{(n+1)} = L^{(n)} \bullet G_{B_{n+1}} \quad (4.3)$$

with the starting condition

$$L^{(1)} = G_{B_1}. \quad (4.4)$$

Here “ \bullet ” denotes the antisymmetric product with multiple groups of antisymmetric indices as defined in equation (3.6). In general G_{B_n} can be a different tensor describing a different type of baryon for each n . The objects G_{B_i} are products of ε -tensors and Γ -matrices and are therefore often sparse. Hence the evaluation of the above recursion can be done very efficiently if only the nonzero components are stored.

According to eqn. (2.5) the correlation function for a given gauge configuration is obtained by evaluating the contraction of L with the product

$$\begin{aligned} F^{(N)}(\delta_1, \dots, \delta_N; t; \xi_1^{(q_1)}, \xi_2^{(q_2)}, \xi_3^{(q_3)}, \dots, \xi_{3N-2}^{(q_1)}, \xi_{3N-1}^{(q_2)}, \xi_{3N}^{(q_3)}) \\ := f_{B_1}^{q_1, q_2, q_3}(t, \delta_1; \xi_1^{(q_1)}, \xi_2^{(q_2)}, \xi_3^{(q_3)}) \dots f_{B_N}^{q_1, q_2, q_3}(t, \delta_N; \xi_{3N-2}^{(q_1)}, \xi_{3N-1}^{(q_2)}, \xi_{3N}^{(q_3)}). \end{aligned} \quad (4.5)$$

³The generalization to systems with additional quark flavors is straightforward. For notational convenience we restrict ourself here to only u -, d - and s -quarks.

To do so one could in principle construct all the components of L explicitly. However, it is computationally more efficient to exploit the antisymmetry of L directly: The tensor F can be projected to a tensor F_- which is antisymmetric in all indices corresponding to the same quark flavor or the same baryon. Only this antisymmetric projection contributes to the correlation function, and therefore, only the contraction between L and F_- has to be evaluated.

F_- possesses the same antisymmetry structure as L , thus it can be written in the form

$$F_-^{(n)}(\mathbf{A}^{(B_a)}\{\delta\}, \mathbf{A}^{(B_b)}\{\delta\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \mathbf{A}^{(d)}\{\xi\}, \mathbf{A}^{(s)}\{\xi\}). \quad (4.6)$$

Since F_- is composed of the independent factors $f_B^{q_1, q_2, q_3}$, a similar recursion relation

$$F_-^{(n+1)} = F_-^{(n)} \bullet f_{B_{n+1}}^{q_1, q_2, q_3} \quad (4.7)$$

with the starting condition $F_-^{(1)} = f_{B_1}^{q_1, q_2, q_3}$ can be defined. In order to apply the above recursion relation one has to calculate explicitly the independent antisymmetric components of $f_{B_i}^{q_1, q_2, q_3}$ by applying all possible permutations of the combined spinor-color indices. Since there are only three such indices in each factor, the computational effort associated with these antisymmetrizations can be neglected compared to the evaluation of the recursion steps of (4.7).

Once both F_- and L are ready, the correlation function can be extracted by performing the contraction

$$\begin{aligned} C^{(N)}(t; \mathbf{A}^{(B_a)}\{\delta\}, \dots, \mathbf{A}^{(u)}\{\alpha\}, \dots) \\ = \frac{1}{\mathcal{N}} \sum_{\substack{\mathbf{A}^{(q_i)}\{\xi\} \\ i \in \{a, b, c\}}} F_-^{(N)}(\mathbf{A}^{(B_a)}\{\delta\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \dots) \cdot L^{(N)}(\mathbf{A}^{(B_a)}\{\alpha\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \dots) \end{aligned} \quad (4.8)$$

with the normalization factor

$$\mathcal{N} = n_{q_a}! n_{q_b}! \dots (n_{B_a}! n_{B_b}! \dots)^2, \quad (4.9)$$

where n_{q_i} is the number of quarks of flavor q_i and n_{B_i} is the number of baryons of type B_i in the system.

The final result $C^{(N)}(\mathbf{A}^{(B_a)}\{\delta\}, \dots, \mathbf{A}^{(u)}\{\alpha\}, \dots)$ itself is an antisymmetric tensor. All components can be reconstructed by taking into account the respective permutations to change the ordering of the indices.

Due to the sparse nature of G_{B_i} the computational cost of the determination of $L^{(N)}$ is very low. Furthermore, this construction has to be performed only once independent of any gauge configuration. The calculation of $F_-^{(m)}$, $m = 1, 2, \dots, N$ is computationally much more demanding and has to be performed on each gauge configuration. The

maximal number of components at the intermediate stage $F_-^{(m)}$ is given by the formula

$$P(n_{B_1}^{(m)}, n_{B_2}^{(m)}, \dots) = \prod_i C(n_{B_i}^{(m)}, 4 - n_{B_i}^{(m)}) \prod_j C(n_{q_j}^{(m)}, 12 - n_{q_j}^{(m)}), \quad (4.10)$$

where $n_{B_i}^{(m)}$ is the number of baryons B_i at the intermediate stage m and $n_{q_j}^{(m)}$ is the number of quarks of flavor q_j at this stage.

In a similar way the maximal number of operations required for adding the baryon B_k in the recursion step $F_-^{(m)} \rightarrow F_-^{(m+1)}$ is

$$Q_{B_k}(n_{B_1}^{(m)}, n_{B_2}^{(m)}, \dots) = \prod_i \begin{cases} C(n_{B_i}^{(m)}, 0, 4 - n_{B_i}^{(m)}) & \text{for } i \neq k \\ C(n_{B_i}^{(m)}, 1, 4 - 1 - n_{B_i}^{(m)}) & \text{for } i = k \end{cases} \times \prod_j \begin{cases} C(n_{q_j}^{(m)}, 0, 12 - n_{q_j}^{(m)}) & \text{for } j \neq k \\ C(n_{q_j}^{(m)}, N(q_j, B_k), 12 - n_{q_j}^{(m)} - N(q_j, B_k)) & \text{for } j = k, \end{cases} \quad (4.11)$$

where $N(q_j, B_k)$ is the number of quarks of flavor q_j in the baryon of type B_k . Formulae (4.10) and (4.11) are special cases of the more general relations (3.7a) and (3.7b).

The estimates P and Q obtained above are only upper bounds on the real computational cost. Due to the large number of zero components of $L^{(N)}$ large savings in comparison with these numbers are possible. During the recursive constructions of $F_-^{(1)}, F_-^{(2)}, \dots, F_-^{(N)}$ only those components have to be calculated, which in the end contribute to a component contracted with a nonzero component of $L^{(N)}$. To do so one calculates the lists $\Lambda^{(1)}, \Lambda^{(2)}, \dots, \Lambda^{(N-1)}$ using the procedure described in Section 3. Then only these operations have to be performed for each gauge configuration.

5 Projection to angular momentum states

The procedure described in the previous section allows the generation of all spinor components of the correlation function. However, in many cases not all spinor components are of interest, but the correlation function is to be projected to a definite angular momentum state. It is often the case that not all components contribute to this projection and hence one wants to avoid the unnecessary computational effort.

Let \mathcal{M} be an arbitrary tensor that projects the correlation function to the required spin state such that

$$C_{\mathcal{M}}(t) = \mathcal{M}_{\delta_1, \delta_2, \dots, \delta_N}^{\alpha_1, \alpha_2, \dots, \alpha_N} [C^{(N)}]_{\delta_1, \delta_2, \dots, \delta_N}^{\alpha_1, \alpha_2, \dots, \alpha_N}(t) \quad (5.1)$$

is the desired projected correlation function. The correlation function $C^{(N)}(t)$ is a tensor with antisymmetric groups of indices, hence only the antisymmetric part of \mathcal{M}

contributes to the resulting correlation function $C_{\mathcal{M}}(t)$. This antisymmetric part can be written as

$$\mathcal{M}_-(\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \dots, \mathbf{A}^{(B_a)}\{\delta\}, \mathbf{A}^{(B_b)}\{\delta\}, \dots) \quad (5.2)$$

and a modified list

$$\begin{aligned} & (n_{B_a}! n_{B_b}! \dots)^2 L_{\mathcal{M}}(\mathbf{A}^{(B_a)}\{\delta\}, \mathbf{A}^{(B_b)}\{\delta\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \mathbf{A}^{(d)}\{\xi\}, \mathbf{A}^{(s)}\{\xi\}) \\ &= \sum_{\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \dots} L^{(N)}(\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \mathbf{A}^{(d)}\{\xi\}, \mathbf{A}^{(s)}\{\xi\}) \\ & \quad \times \mathcal{M}_-(\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \dots, \mathbf{A}^{(B_a)}\{\delta\}, \mathbf{A}^{(B_b)}\{\delta\}, \dots) \end{aligned} \quad (5.3)$$

can be defined. Then this modified list can be used to calculate the projected correlation function

$$C_{\mathcal{M}}(t) = \frac{1}{\mathcal{N}} \sum_{\mathbf{A}} F_{-}^{(N)}(\mathbf{A}^{(B_a)}\{\delta\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \dots) \cdot L_{\mathcal{M}}(\mathbf{A}^{(B_a)}\{\delta\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \dots). \quad (5.4)$$

Here the sum goes over all tuples of antisymmetric sets of indices. Only those components of $F_{-}^{(N)}$ contribute to the correlation function for which the corresponding component of $L_{\mathcal{M}}^{(N)}$ is nonzero. The number of contributing components is always smaller or equal to the number of components that would be necessary to evaluate if the complete correlation function were of interest. This fact can be exploited in the generation of the lists of operations $\Lambda^{(1)}, \Lambda^{(2)}, \dots, \Lambda^{(N)}$.

6 Multiple sources/sinks

In the previous sections the number of quark sources was set to one. In this case due to the Pauli-principle the maximal number of baryons is restricted in such a way that only 12 quarks of each flavor are allowed in the system. This restriction can be circumvented by introducing additional quark sources. When we have N_s mutually orthogonal quark sources, an additional source-index s ranging from 1 to N_s can be introduced to each quark operator. Then the baryon operators at the source also have to be modified accordingly,

$$\bar{B}^{\alpha;s} = \varepsilon^{abc} (\Gamma_1)^{\alpha\beta} (\bar{q}_1)^{\beta;a;s} [(\bar{q}_2)^{\gamma;b;s} (\Gamma_2)^{\gamma\delta} (\bar{q}_3)^{\delta;c;s}]. \quad (6.1)$$

As a consequence, the generation of the objects G^B has to be modified in such a way that the fact that all quarks of a baryon originate from the same source is respected.⁴ This can be achieved by the straightforward modification: the indices $\xi^{(q_i)}$ are promoted

⁴Although this restriction is not necessary for the algorithm described here, it is introduced to keep our notation simple and to allow for a cleaner presentation of the algorithm. The generalization to other cases is straightforward.

to combined spinor-color-source indices which range from 1 to $12N_s$. Then the modified \tilde{G}^B becomes

$$\tilde{G}^B(\alpha, s; \xi^{(q_1)}, \xi^{(q_2)}, \xi^{(q_3)}) := \delta^{s, s(\xi^{(q_1)})} \delta^{s, s(\xi^{(q_2)})} \delta^{s, s(\xi^{(q_3)})} G^B(\alpha; \kappa(\xi^{(q_1)}), \kappa(\xi^{(q_2)}), \kappa(\xi^{(q_3)})), \quad (6.2)$$

where $s(\xi)$ is the source part of the combined index ξ and $\kappa(\xi)$ is the spinor-color part of ξ . The sink part also needs to be modified by using different sink functions $s_1(\vec{x}), s_2(\vec{x}), \dots$ in the generation of the blocks $f_B^{q_1, q_2, q_3}(t, \delta; \alpha, \beta, \gamma; a, b, c)$.

To simplify the notation combined spinor-source indices χ and ψ can be introduced to replace the former spinor indices of the baryons at the source and at the sink, respectively. Thus, the objects \tilde{G} and the modified blocks $\tilde{f}_B^{q_1, q_2, q_3}$ can be written as

$$\begin{aligned} \tilde{G}^B(\chi; \xi^{(q_1)}, \xi^{(q_2)}, \xi^{(q_3)}) &= \delta^{s(\chi), s(\xi^{(q_1)})} \delta^{s(\chi), s(\xi^{(q_2)})} \delta^{s(\chi), s(\xi^{(q_3)})} \\ &\quad \cdot G^B(\alpha(\chi); \kappa(\xi^{(q_1)}), \kappa(\xi^{(q_2)}), \kappa(\xi^{(q_3)})), \end{aligned} \quad (6.3)$$

$$\tilde{f}_B^{q_1, q_2, q_3}(t, \psi; \xi^{(q_1)}, \xi^{(q_2)}, \xi^{(q_3)}) = \sum_{\vec{x}} s_{s(\psi)}(\vec{x}) \left\langle B_{\alpha(\psi)}(\vec{x}, t) \cdot q_1^{\xi^{(q_1)}} q_2^{\xi^{(q_2)}} q_3^{\xi^{(q_3)}} \right\rangle. \quad (6.4)$$

Here $s(\chi)$ is the source part of the index χ , $s(\psi)$ is the sink part of the index ψ , and $\alpha(\chi)$ and $\alpha(\psi)$ are the spinor parts of the indices χ and ψ , respectively.

The recursion relations (4.3) and (4.7) for L and F_- remain valid with the only difference that $\tilde{f}_B^{q_a, q_b, q_c}$ and \tilde{G}_B are used instead of $f_B^{q_a, q_b, q_c}$ and G_B . The correlation function can be calculated similarly to (4.8) by evaluating the contraction

$$\begin{aligned} C^{(N)}(t; \mathbf{A}^{(B_a)}\{\psi\}, \dots, \mathbf{A}^{(u)}\{\chi\}, \dots) \\ = \frac{1}{\mathcal{N}} \sum_{\substack{\mathbf{A}^{(q_i)}\{\xi\} \\ i \in \{a, b, c\}}} F_-^{(N)}(\mathbf{A}^{(B_a)}\{\psi\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \dots) \cdot L^{(N)}(\mathbf{A}^{(B_a)}\{\chi\}, \dots, \mathbf{A}^{(u)}\{\xi\}, \dots). \end{aligned} \quad (6.5)$$

Here the only difference is that the result $C^{(N)}(t; \mathbf{A}^{(B_a)}\{\psi\}, \dots, \mathbf{A}^{(u)}\{\chi\}, \dots)$ instead of only spin indices now possesses combined source/sink-spinor indices.

The upper bounds for the computational effort for the construction of the tensors F_- can be generalized in a straightforward way to

$$P(n_{B_1}^{(m)}, n_{B_2}^{(m)}, \dots) = \prod_i C(n_{B_i}^{(m)}, 4N_s - n_{B_i}^{(m)}) \prod_j C(n_{q_j}^{(m)}, 12N_s - n_{q_j}^{(m)}) \quad (6.6)$$

and

$$Q_{B_k}(n_{B_1}^{(m)}, n_{B_2}^{(m)}, \dots) = \prod_i \begin{cases} C(n_{B_i}^{(m)}, 0, 4N_s - n_{B_i}^{(m)}) & \text{for } i \neq k \\ C(n_{B_i}^{(m)}, 1, 4N_s - 1 - n_{B_i}^{(m)}) & \text{for } i = k \end{cases} \\ \times \prod_j \begin{cases} C(n_{q_j}^{(m)}, 0, 12N_s - n_{q_j}^{(m)}) & \text{for } j \neq k \\ C(n_{q_j}^{(m)}, N(q_j, B_k), 12N_s - n_{q_j}^{(m)} - N(q_j, B_k)) & \text{for } j = k. \end{cases} \quad (6.7)$$

7 Atomic nuclei

In this section the important special case of atomic nuclei, that is, systems consisting of protons and neutrons is discussed. For the calculation the nucleon operators

$$P_\alpha = \varepsilon_{abc} (\Gamma_1)_{\alpha\beta} u_{\beta;a} [u_{\gamma;b} (\Gamma_2)_{\gamma\delta} d_{\delta;c}], \quad (7.1a)$$

$$N_\alpha = \varepsilon_{abc} (\Gamma_1)_{\alpha\beta} d_{\beta;a} [u_{\gamma;b} (\Gamma_2)_{\gamma\delta} d_{\delta;c}] \quad (7.1b)$$

are used at the sink and the operators

$$\bar{P}^\alpha = \varepsilon^{abc} (\Gamma_1)_{\alpha\beta} \bar{u}^{\beta;a} [\bar{u}^{\gamma;b} (\Gamma_2)_{\gamma\delta} \bar{d}^{\delta;c}], \quad (7.1c)$$

$$\bar{N}^\alpha = \varepsilon^{abc} (\Gamma_1)^{\alpha\beta} \bar{d}^{\beta;a} [\bar{u}^{\gamma;b} (\Gamma_2)_{\gamma\delta} \bar{d}^{\delta;c}] \quad (7.1d)$$

are used at the source. There are two common choices for the set of matrices (Γ_1, Γ_2) . The first choice, $\Gamma_1 = \mathbf{1}$ and $\Gamma_2 = C\gamma_5$, where C is the charge conjugation matrix, gives fully relativistic nucleon operators. In case of the second choice, $\Gamma_1 = P_{nr}$ and $\Gamma_2 = C\gamma_5 P_{nr}$, the projection $P_{nr} = (1 + \gamma_4)/2$ to the “non-relativistic” spinor components is inserted. In this case, if the Dirac representation of the γ -matrices is used, only the upper two spinor components contribute to the operators. Therefore, by using non-relativistic operators the computational effort can be reduced significantly.

Introducing the variables n_P and n_N to denote the number of protons and neutrons in the system, the recursion relations of adding one proton or one neutron can be written as

$$L^{(n_P+1, n_N)} = L^{(n_P, n_N)} \bullet G_P, \quad (7.2a)$$

$$L^{(n_P, n_N+1)} = L^{(n_P, n_N)} \bullet G_N, \quad (7.2b)$$

$$F_-^{(n_P+1, n_N)} = F_-^{(n_P, n_N)} \bullet f_P^{u,u,d}, \quad (7.2c)$$

$$F_-^{(n_P, n_N+1)} = F_-^{(n_P, n_N)} \bullet f_N^{d,u,d}, \quad (7.2d)$$

with the starting conditions either

$$L^{(0,1)} = G_N \quad \text{and} \quad F_-^{(0,1)} = f_N^{d,u,d} \quad (7.3a)$$

or

$$L^{(1,0)} = G_P \quad \text{and} \quad F_-^{(1,0)} = f_P^{u,u,d}. \quad (7.3b)$$

The upper bound for the number of components of F_- at each stage is

$$P(n_P, n_N) = C(n_P, D - n_P)C(n_N, D - n_N) \\ C(2n_P + n_N, 3D - 2n_P - n_N)C(n_P + 2n_N, 3D - n_P - 2n_N), \quad (7.4)$$

where D denotes the effective number of spinor components. For relativistic operators $D = 4$ and for non-relativistic operators $D = 2$. The upper bounds for the number of operations to add a proton or a neutron to $F_-^{(n_P, n_N)}$ are

$$Q_P(n_P, n_N) = (n_P, 1, D - 1 - n_P)C(n_N, D - n_N)C(2n_P + n_N, 2, 3D - 2 - 2n_P - n_N) \\ C(n_P + 2n_N, 1, 3D - 1 - n_P - 2n_N), \quad (7.5a)$$

$$Q_N(n_P, n_N) = (n_P, D - n_P)C(n_N, 1, D - 1 - n_N)C(2n_P + n_N, 1, 3D - 1 - 2n_P - n_N) \\ C(n_P + 2n_N, 2, 3D - 2 - n_P - 2n_N). \quad (7.5b)$$

To calculate the tensor $F_-^{(N_P, N_N)}$ for fixed values of N_P and N_N one can choose several different orders of the recursion operations (7.2a–7.2d). One could for example start with adding only neutrons until $F_-^{(0, N_N)}$ is reached and then start to add only protons until the final result $F_-^{(N_P, N_N)}$ is obtained. For a first estimate of which order is best the values of the function $P(n_P, n_N)$ at the intermediate stages can be used. Figure 2 gives these values for relativistic operators and compares two possible “paths” leading to the same state. It can be seen that for a given $A = n_N + n_P$ the tensors with a minimal number of components correspond to $A = n_N$ or $A = n_P$. After investigating $Q_P(n_P, n_N)$ and $Q_N(n_P, n_N)$ it was found that the estimated operation count is minimal when first all the baryons of one type, e.g. neutrons, are added before adding any of the other type. Several different paths for several different nuclei have been tried numerically and it was found that even with the reduction due to the not required components these paths were still the most efficient in all tested cases.

The lists of operations $\Lambda_P^{(n_P, n_N)}$ and $\Lambda_N^{(n_P, n_N)}$ for the addition of protons or neutrons to $F_-^{(n_P, n_N)}$ have been constructed explicitly for a broad range of nuclei. These lists are different for each choice of the numbers N_P and N_N even for the same intermediate stages (n_P, n_N) due to the fact that different components can be ignored depending on N_P and N_N . In each case the path corresponding to adding the N_N neutrons before the addition of the N_P protons was chosen. The generation of the lists takes less than an hour on a standard desktop computer for all nuclei accessible with one quark source and relativistic operators. In the non relativistic case the generation of the lists takes less than 0.1 seconds on the same computer.

The computational effort of generating the correlation functions of atomic nuclei is dominated by the operations necessary to construct the tensors F_- . All other computational

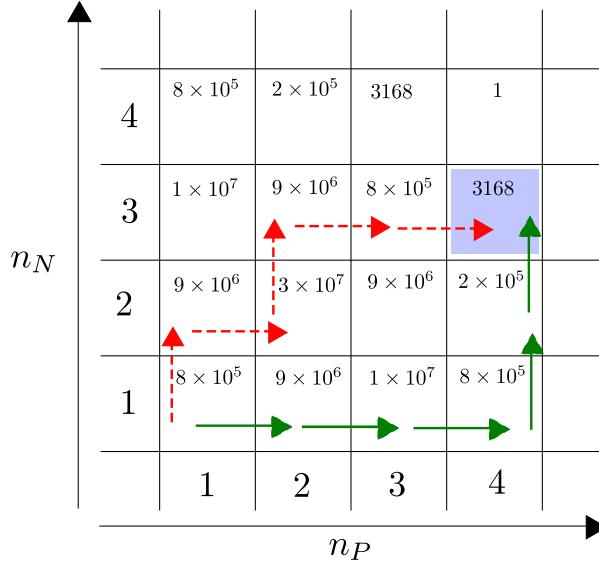


Figure 2: Two possible paths for the recursion relation to reach $F_-^{(4,3)}$ in the case of relativistic operators. The green (solid) path is more efficient than the red (dashed) path. The numbers in each box are the values of $P(n_P, n_N)$, that is, the upper bound for the number of components of $F_-^{(n_P, n_N)}$.

tasks, such as the summation in equation (4.8) or the construction of $f_P^{u,u,d}$ and $f_N^{d,u,d}$ can be neglected. Table 1 shows the number of operations required for the construction of atomic nuclei with one quark source and relativistic operators. Here each operation is an element of a list Λ required for the given nucleus and amounts to a complex addition and multiplication. The numbers are also compared to the naïve numbers of operations that would be required if one evaluated all Wick-contractions and spinor and color loops. The same information for the case of non-relativistic operators is shown in Table 2. A calculation with non-relativistic operators and two quark sources according to Section 6 was also performed. The resulting numbers of operations are shown in Table 3.

These numbers show that the calculation of the correlation function of atomic nuclei using the recursive approach discussed in this paper is by many orders of magnitude more efficient than the naive computation.

8 Comparison of efficiency

In this section we compare the efficiency of the procedure described in the previous sections with the unified contraction algorithm introduced in Ref. [8] and the determinant method introduced in Ref. [7].

The method of Ref. [8] requires the construction of a unified list of contractions. This

list is identical to the tensor $L^{(N_P, N_N)}$ used in this paper except that it is not stored in an antisymmetrized form. Hence the number of entries N_{list} is by a factor $n_u! n_d! n_s!$ larger than the number of entries in $L^{(N_P, N_N)}$. The generation of the unified contraction list in Ref. [8] is done by explicitly applying all possible permutations of quark indices. The effort associated with these permutations scales with $n_u! n_d! n_s!$ and even for systems of moderate sizes the generation of the list requires supercomputers. In contrast to this our recursive construction of the similar objects L requires about a second on todays desktop computers for all nuclei accessible with one quark source and relativistic operators.

Once the list is generated the number of evaluations of $f_B^{(q_1, q_2, q_3)}$ required on each gauge configuration is $AN_{\text{list}}/2^A = AN_{\text{contr}}$. In our approach the number of evaluations of $f_B^{(q_1, q_2, q_3)}$ is equal to the number of elements N_{Λ} in the operation list Λ required for the recursion. Therefore, the ratio of the efficiency of our algorithm and that of the unified contraction algorithm can be roughly estimated as $AN_{\text{contr}}/N_{\Lambda}$.

To be able to compare our method with the performance numbers listed in Ref. [8] the different spin components have to be computed separately. We stress that this is less efficient than calculating all components at once if one is interested in all components. Individual spin components can be computed using the technique described in Section 5. If the spin indices of the desired component are $(\gamma_1, \gamma_2, \dots, \gamma_A)$ at the source and $(\gamma'_1, \gamma'_2, \dots, \gamma'_A)$ at the sink then the projection tensor

$$\mathcal{M}_{\delta_1 \delta_2 \dots \delta_A}^{\alpha_1 \alpha_2 \dots \alpha_A} = \delta^{\delta_1 \gamma_1} \delta^{\delta_2 \gamma_2} \dots \delta^{\delta_A \gamma_A} \delta_{\alpha_1 \gamma'_1} \delta_{\alpha_2 \gamma'_2} \dots \delta_{\alpha_A \gamma'_A} \quad (8.1)$$

is to be used. Since only the choice for the spin component at the source enters the calculation of the correlation function one can choose $\gamma_i = \gamma'_i$ for the efficiency comparison.

Table 4 shows the comparison between our method and the unified contraction algorithm in the non-relativistic case. Table 5 presents the same comparison in the case of relativistic operators. In Table 6 the efficiency in the case of non-relativistic operators and two quark sources is shown. For the sake of readability not all components are tabulated in the case of relativistic operators. More precisely only components with the minimal possible number of lower half spinor indices are listed. This includes all non-zero components calculated in Ref. [8]. The computational effort associated with the components not listed is in all cases of the same order of magnitude as the listed components with the same N_P and N_N .

The method of Ref. [7] uses determinants for the calculation of the quark level permutations in the correlation function for a fixed structure of color-/spinor-indices and spatial location of the operators at the source and at the sink. This algorithm scales as

$$n_u^3 n_d^3 n_s^3 \cdot N_w N'_w, \quad (8.2)$$

where N_w and N'_w are the number of such independent structures up to permutations of quarks at the source and at the sink, respectively. This algorithm is especially efficient

in the case where the numbers of quarks n_u , n_d and n_s are chosen such that all possible spinor- and color-DoFs are fully saturated both at the source and at the sink. In this case $N_w = N'_w = 1$. Such combinations of operators can be found for the nuclei ${}^4\text{He}$, ${}^8\text{Be}$, ${}^{12}\text{C}$, ${}^{16}\text{O}$ and ${}^{28}\text{Si}$ for which concrete results are presented in Ref. [7]. However, in the general case the numbers N_w and N'_w may become very large and in fact scale exponentially as already noted in Ref. [7].

If the individual baryons are to have a complex spatial structure, which is required e.g. for the projection to a definite momentum and angular momentum, it is very difficult to find a combination of operators for which N_w and N'_w remain small. In such cases the algorithm presented in this paper, which can perform the construction of baryon blocks with complex spatial structure in advance of the calculation, can be more advantageous.

9 Summary

We introduced a procedure to compute the correlation functions of multi-baryon systems using a recursive technique. In a first step a list of required components is generated in a recursive manner, where several antisymmetry properties of the list are exploited. In a second step a product of blocks of quark propagators is constructed recursively on each gauge configuration. During the construction both the antisymmetry of this product and the reduction due to the sparse nature of the list of required components are exploited at each intermediate step.

The individual baryons in the system can be projected to any momentum state prior to the calculation, e.g. to zero momentum to extract the ground state mass. Different quark sources and baryon sinks can be used to create correlation functions with spatial structure and an arbitrary number of baryons in the system. The procedure can be employed for a broad range of multi-baryon systems. Systems with quantum numbers of atomic nuclei were discussed in detail.

Our technique was compared in detail with the naïve method and the method proposed in [8] and it was found that a significant speedup in all cases with $A > 2$ is possible. For the construction of the ${}^4\text{He}$ and ${}^8\text{Be}$ correlation functions with relativistic operators $\mathcal{O}(10^8)$ operations are required. In the non-relativistic approximation for ${}^4\text{He}$ the required number of operations is only $\mathcal{O}(10^4)$.

References

- [1] **PACS-CS** Collaboration, T. Yamazaki, Y. Kuramashi, and A. Ukawa, *Helium Nuclei in Quenched Lattice QCD*, *Phys. Rev.* **D81** (2010) 111504, [[arXiv:0912.1383](https://arxiv.org/abs/0912.1383)].

- [2] S. Beane, E. Chang, S. Cohen, W. Detmold, H. Lin, *et. al.*, *Light Nuclei and Hypernuclei from Quantum Chromodynamics in the Limit of SU(3) Flavor Symmetry*, [arXiv:1206.5219](https://arxiv.org/abs/1206.5219).
- [3] T. Yamazaki, K.-I. Ishikawa, Y. Kuramashi, and A. Ukawa, *Helium nuclei, deuteron and dineutron in 2+1 flavor lattice QCD*, *Phys.Rev.* **D86** (2012) 074514, [[arXiv:1207.4277](https://arxiv.org/abs/1207.4277)].
- [4] N. Ishii, S. Aoki, and T. Hatsuda, *The Nuclear Force from Lattice QCD*, *Phys.Rev.Lett.* **99** (2007) 022001, [[nucl-th/0611096](https://arxiv.org/abs/nucl-th/0611096)].
- [5] S. Aoki, T. Hatsuda, and N. Ishii, *Theoretical Foundation of the Nuclear Force in QCD and its applications to Central and Tensor Forces in Quenched Lattice QCD Simulations*, *Prog.Theor.Phys.* **123** (2010) 89–128, [[arXiv:0909.5585](https://arxiv.org/abs/0909.5585)].
- [6] **HAL QCD** Collaboration, T. Doi *et. al.*, *Exploring Three-Nucleon Forces in Lattice QCD*, *Prog.Theor.Phys.* **127** (2012) 723–738, [[arXiv:1106.2276](https://arxiv.org/abs/1106.2276)].
- [7] W. Detmold and K. Orginos, *Nuclear correlation functions in lattice QCD*, [arXiv:1207.1452](https://arxiv.org/abs/1207.1452).
- [8] T. Doi and M. G. Endres, *Unified contraction algorithm for multi-baryon correlators on the lattice*, [arXiv:1205.0585](https://arxiv.org/abs/1205.0585).
- [9] W. Detmold and M. J. Savage, *A method to study complex systems of mesons in Lattice QCD*, *Phys.Rev.* **D82** (2010) 014511, [[arXiv:1001.2768](https://arxiv.org/abs/1001.2768)].

Table 1: Number of operations (each operation is a complex multiplication and addition) required to compute all independent spinor components of the correlation function with N_P protons and N_N neutrons with one quark source and relativistic operators. Both the naïve number and the number using the recursive approach are given. η is the gain factor, that is, the ratio of the naïve and the recursive numbers of operations.

N_P	N_N	No. of op.	Naïve No. of op.	η
0	2	199584	15925248	79.8
0	3	5825088	8.3×10^{11}	1.4×10^5
0	4	54768672	1.1×10^{17}	1.9×10^9
1	1	474048	11943936	25.2
1	2	19241280	5.5×10^{11}	2.9×10^4
1	3	109789200	6.7×10^{16}	6.1×10^8
1	4	179769600	1.7×10^{22}	9.2×10^{13}
2	2	531321120	5.7×10^{16}	1.1×10^8
2	3	756897264	1.3×10^{22}	1.7×10^{13}
2	4	291957888	5.3×10^{27}	1.8×10^{19}
3	3	2905079520	4.9×10^{27}	1.7×10^{18}
3	4	404946240	3.0×10^{33}	7.5×10^{24}
4	4	448496928	2.8×10^{39}	6.2×10^{30}

Table 2: Number of operations (each operation is a complex multiplication and addition) required to compute all independent spinor components of the correlation function with N_P protons and N_N neutrons with one quark source and non-relativistic operators. Both the naïve number and the number using the recursive approach are given. η is the gain factor, that is, the ratio of the naïve and the recursive numbers of operations.

N_P	N_N	No. of op.	Naïve No. of op.	η
0	2	504	995328	1974.9
1	1	2664	746496	280.2
1	2	6048	8.6×10^9	1.4×10^6
2	2	10980	2.2×10^{14}	2.0×10^{10}

Table 3: Number of operations (each operation is a complex multiplication and addition) required to compute all independent spinor components of the correlation function with N_P protons and N_N neutrons with two quark sources and non-relativistic operators. Both the naïve number and the number using the recursive approach are given. η is the gain factor, that is, the ratio of the naïve and the recursive numbers of operations.

N_P	N_N	No. of op.	Naïve No. of op.	η
0	2	3024	995328	329.1
0	3	1052136	1.3×10^{10}	1.2×10^4
0	4	18881568	4.2×10^{14}	2.2×10^7
1	1	10656	746496	70.1
1	2	42768	8.6×10^9	2.0×10^5
1	3	6329016	2.6×10^{14}	4.1×10^7
1	4	67720680	1.6×10^{19}	2.4×10^{11}
2	2	103680	2.2×10^{14}	2.1×10^9
2	3	10038672	1.3×10^{19}	1.3×10^{12}
2	4	81850128	1.3×10^{24}	1.6×10^{16}
3	3	338263368	1.3×10^{24}	3.5×10^{15}
3	4	287427384	1.9×10^{29}	6.5×10^{20}
4	4	448496928	4.2×10^{34}	9.5×10^{25}

Table 4: The efficiency of the presented algorithm for the calculation of individual spin components with non-relativistic operators. N_Λ is the number of operations (complex multiplications and additions) required for the construction of F_- . N_L is the number of independent components of the tensor L . N_{list} and N_{contr} are the number of entries in the unified contraction list and the number of independent contractions from Ref. [8], respectively. (Numbers that are not presented in [8] are from own calculations). $AN_{\text{contr.}}/N_\Lambda$ is approximately the ratio of the number of operations required for the unified contraction algorithm and for the algorithm presented in this paper if additions are taken as much faster then multiplications.

N_P	N_N	spinstate	N_Λ	N_L	N_{list}	N_{contr}	$AN_{\text{contr.}}/N_\Lambda$
0	2	(0,1)	504	21	1008	252	1
1	1	(0,0)	189	21	756	189	2
1	1	(1,0)	252	28	1008	252	2
1	1	(0,1)	252	28	1008	252	2
1	1	(1,1)	189	21	756	189	2
1	2	(0,0,1)	4662	9	25920	3240	2.1
1	2	(1,0,1)	4662	9	25920	3240	2.1
2	2	(0,1,0,1)	10980	1	518400	32400	11.8

Table 5: The efficiency of the presented algorithm for the calculation of individual spin components with relativistic operators. N_Λ is the number of operations (complex multiplications and additions) required for the construction of F_- . N_L is the number of independent components of the tensor L . N_{list} and N_{contr} are the number of entries in the unified contraction list and the number of independent contractions from Ref. [8], respectively. (Numbers that are not presented in [8] are from own calculations). $\text{AN}_{\text{contr.}}/N_\Lambda$ is approximately the ratio of the number of operations required for the unified contraction algorithm and for the algorithm presented in this paper if additions are taken as much faster then multiplications.

N_P	N_N	spinstate	N_Λ	N_L	N_{list}	N_{contr}	$\text{AN}_{\text{contr.}}/N_\Lambda$
0	2	(0,1)	5544	231	11088	2772	1
0	3	(0,1,2)	1360098	1110	4795200	599400	1.3
0	3	(0,1,3)	1360098	1110	4795200	599400	1.3
0	4	(0,1,2,3)	54768672	1845	1785369600	111585600	8.1
1	1	(0,0)	2079	231	8316	2079	2
1	1	(1,0)	2358	262	9432	2358	2
1	1	(0,1)	2358	262	9432	2358	2
1	1	(1,1)	2079	231	8316	2079	2
1	2	(0,0,1)	381978	1311	3775680	471960	3.7
1	2	(1,0,1)	381978	1311	3775680	471960	3.7
1	3	(0,0,1,2)	11717937	2232	1349913600	84369600	28.8
1	3	(1,0,1,2)	11717937	2232	1349913600	84369600	28.8
1	3	(0,0,1,3)	11717937	2232	1349913600	84369600	28.8
1	3	(1,0,1,3)	11717937	2232	1349913600	84369600	28.8
1	4	(0,0,1,2,3)	141103602	1110	290013696000	9062928000	321.1
1	4	(1,0,1,2,3)	141103602	1110	290013696000	9062928000	321.1
2	2	(0,1,0,1)	8541864	2716	1407974400	87998400	41.2
2	3	(0,1,0,1,2)	44343561	1311	266411980800	8325374400	938.7
2	3	(0,1,0,1,3)	44343561	1311	266411980800	8325374400	938.7
2	4	(0,1,0,1,2,3)	214572144	231	33798352896000	528099264000	14767
3	3	(0,1,2,0,1,2)	163007703	231	30418517606400	475289337600	17494.5
3	3	(0,1,3,0,1,2)	181280493	262	34500656332800	539072755200	17842.2
3	3	(0,1,2,0,1,3)	181280493	262	34500656332800	539072755200	17842.2

Table 5: The efficiency of the presented algorithm for the calculation of individual spin components with relativistic operators. N_Λ is the number of operations (complex multiplications and additions) required for the construction of F_- . N_L is the number of independent components of the tensor L . N_{list} and N_{contr} are the number of entries in the unified contraction list and the number of independent contractions from Ref. [8], respectively. (Numbers that are not presented in [8] are from own calculations). $AN_{\text{contr.}}/N_\Lambda$ is approximately the ratio of the number of operations required for the unified contraction algorithm and for the algorithm presented in this paper if additions are taken as much faster then multiplications.

N_P	N_N	spinstate	N_Λ	N_L	N_{list}	N_{contr}	$AN_{\text{contr.}}/N_\Lambda$
3	3	(0,1,3,0,1,3)	163007703	231	30418517606400	475289337600	17494.5
3	4	(0,1,2,0,1,2,3)	293717796	21	3041851760640000	23764466880000	566364
3	4	(0,1,3,0,1,2,3)	293717796	21	3041851760640000	23764466880000	566364
4	4	(0,1,2,3,0,1,2,3)	448496928	1	22942532802560000	896259893760000	1.6×10^7

Table 6: The efficiency of the presented algorithm for the calculation of individual spin components with non-relativistic operators using two quark sources. N_Λ is the number of operations (complex multiplications and additions) required for the construction of F_- . N_L is the number of independent components of the tensor L . N_{list} and N_{contr} are the number of entries in the unified contraction list and the number of independent contractions from Ref. [8], respectively. (Numbers that are not presented in [8] are from own calculations). $AN_{\text{contr.}}/N_\Lambda$ is approximately the ratio of the number of operations required for the unified contraction algorithm and for the algorithm presented in this paper if additions are taken as much faster then multiplications. The combined spinor-source indices are of the form $2\alpha + s$ where α is the spinor part and s is the source part.

N_P	N_N	spinor-/source-indices	N_Λ	N_L	N_{list}	N_{contr}	$AN_{\text{contr.}}/N_\Lambda$
0	2	(0,2)	504	21	1008	252	1
0	3	(0,1,2)	330291	189	816480	102060	0.9
0	3	(0,2,3)	330291	189	816480	102060	0.9
0	4	(0,1,2,3)	18881568	441	426746880	26671680	5.7
1	1	(0,0)	189	21	756	189	2
1	1	(2,0)	252	28	1008	252	2
1	1	(0,2)	252	28	1008	252	2
1	1	(2,2)	189	21	756	189	2
1	2	(0,0,2)	4662	9	25920	3240	2.1
1	2	(2,0,2)	4662	9	25920	3240	2.1

Table 6: The efficiency of the presented algorithm for the calculation of individual spin components with non-relativistic operators using two quark sources. N_Λ is the number of operations (complex multiplications and additions) required for the construction of F_- . N_L is the number of independent components of the tensor L . N_{list} and N_{contr} are the number of entries in the unified contraction list and the number of independent contractions from Ref. [8], respectively. (Numbers that are not presented in [8] are from own calculations). $AN_{\text{contr.}}/N_\Lambda$ is approximately the ratio of the number of operations required for the unified contraction algorithm and for the algorithm presented in this paper if additions are taken as much faster then multiplications. The combined spinor-source indices are of the form $2\alpha + s$ where α is the spinor part and s is the source part.

N_P	N_N	spinor-/source-indices	N_Λ	N_L	N_{list}	N_{contr}	$AN_{\text{contr.}}/N_\Lambda$
1	3	(0,0,1,2)	1100034	81	48988800	3061800	11.1
	1	(2,0,1,2)	1100034	81	48988800	3061800	11.1
	1	(0,0,2,3)	1100034	81	48988800	3061800	11.1
	1	(2,0,2,3)	1100034	81	48988800	3061800	11.1
	1	(0,0,1,2,3)	59747247	189	49380710400	1543147200	129.1
	1	(2,0,1,2,3)	59747247	189	49380710400	1543147200	129.1
2	2	(0,2,0,2)	10980	1	518400	32400	11.8
	2	(0,2,0,1,2)	1717569	9	1828915200	57153600	166.4
	2	(0,2,0,2,3)	1717569	9	1828915200	57153600	166.4
	2	(0,2,0,1,2,3)	80357088	21	3072577536000	48009024000	3584.7
	3	(0,1,2,0,1,2)	31373721	21	2765319782400	43208121600	8263.3
	3	(0,2,3,0,1,2)	40214061	28	3687093043200	57610828800	8595.6
	3	(0,1,2,0,2,3)	40214061	28	3687093043200	57610828800	8595.6
	3	(0,2,3,0,2,3)	31373721	21	2765319782400	43208121600	8263.3
	3	(0,1,2,0,1,2,3)	225681807	9	1303650754560000	10184771520000	315902
	3	(0,2,3,0,1,2,3)	225681807	9	1303650754560000	10184771520000	315902
4	4	(0,1,2,3,0,1,2,3)	448496928	1	229442532802560000	896259893760000	1.6×10^7